Biphenyl

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.59e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

Image not found
1-Methoxy-2-nitrobenzene
Measured: 8.93e-03
Predicted: 6.33e-03

Image not found
1-Methylnaphthalene
Measured: 2.90e-02
Predicted: 2.13e-02

Image not found
2-Methylnaphthalene
Measured: 1.22e-02
Predicted: 2.48e-02

Image not found
p-Bromodiphenyl ether
Measured: 8.21e-03
Predicted: 1.93e-03

Image not found
Tripropylamine
Measured: 2.46e-03
Predicted: 4.93